Introduction to Computational Physics PHYS 250 (Autumn 2018) – Lecture 2

David Miller

Department of Physics and the Enrico Fermi Institute University of Chicago

October 4, 2018

Outline

- 🕖 Quick git/GitHub tutorial
 - Basics of git
 - git workflow
 - Our usage of git and GitHub resources
- Plan for homework
 - Using **GitHub** Classroom
- B Physics
 - Random numbers: Introduction and motivation
 - Types of random numbers
 - Hypothesis testing and random numbers

Version control reminders



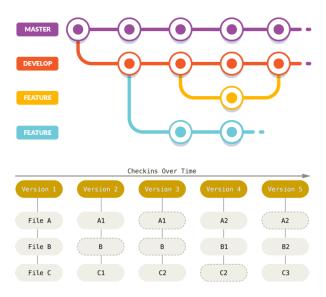
We will be using these tools for the course. There are **many** awesome tutorials out there, and here are a few of my favorite bookmarks:

- "Hello World" from GitHub
- An Intro to Git and GitHub for Beginners (Tutorial)
- A Visual Git Reference
- An Intro to Git and GitHub

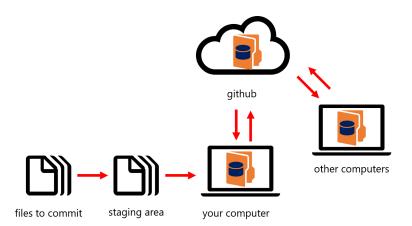
A basic summary of the concept of git, in my words, is:

git takes a snapshot of the entire "project" and saves it, kind of like running Time Machine (or any disk backup) on your entire hard drive every time.

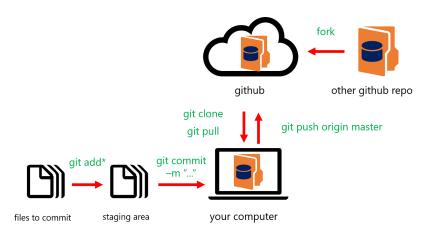
git concept in pictures



What does a git work flow look like?



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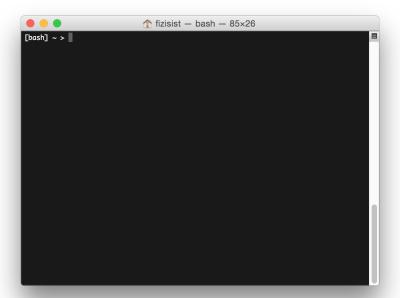


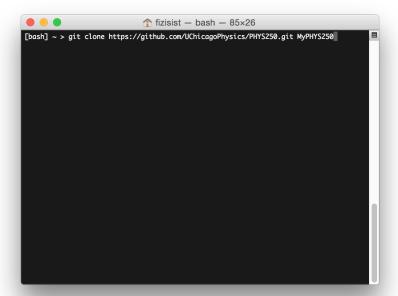
What does a git work flow look like?

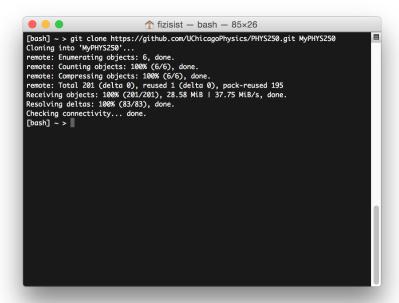
The five commands you use the most are:

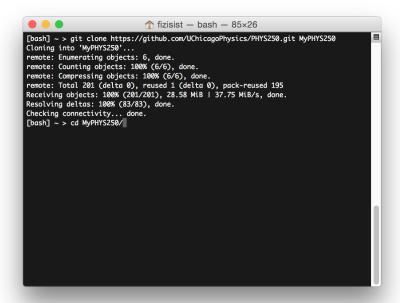
- git add files: copies files (at their current state) to the stage.
- git commit -m "MESSAGE": saves a snapshot of the stage as a commit.
- git reset *files*: copies *files* from the latest commit to the stage.
 - Use this command to "undo" a git add files. You can also git reset to unstage everything.
- git checkout *files*: copies *files* from the stage to the working directory. Use this to throw away local changes.
- git push: send everything in your local repository back to the master



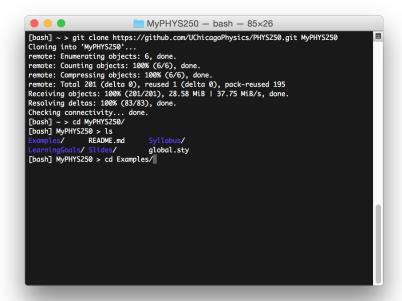


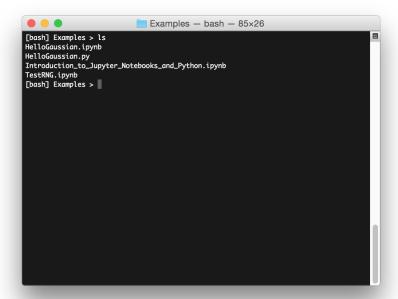




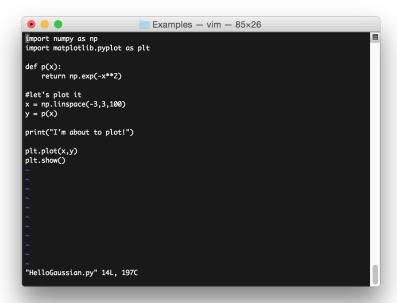


```
MvPHYS250 - bash - 85x26
[bash] ~ > git clone https://github.com/UChicagoPhysics/PHYS250.git MyPHYS250
Cloning into 'MyPHYS250'...
remote: Enumerating objects: 6, done.
remote: Counting objects: 100% (6/6), done.
remote: Compressing objects: 100% (6/6), done.
remote: Total 201 (delta 0), reused 1 (delta 0), pack-reused 195
Receiving objects: 100% (201/201), 28.58 MiB | 37.75 MiB/s, done.
Resolving deltas: 100% (83/83), done.
Checking connectivity... done.
[bash] ~ > cd MyPHYS250/
[bash] MyPHYS250 > 1s
              README.md
LearningGoals/ Slides/
                             global.sty
Γbash | MyPHYS250 > ■
```

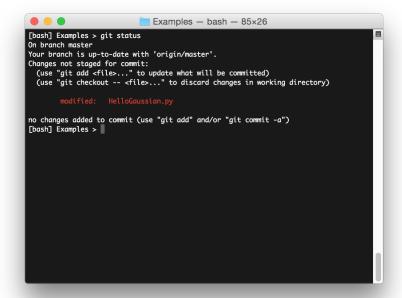




```
Examples - vim - 85×26
import numpy as np
import matplotlib.pyplot as plt
def p(x):
    return np.exp(-x**2)
#let's plot it
x = np.linspace(-3,3,100)
y = p(x)
plt.plot(x,y)
plt.show()
"HelloGaussian.py" [noeol] 11L, 166C
```



```
Examples - bash - 85x26
[bash] Examples > git diff HelloGaussian.py
diff --git a/Examples/HelloGaussian.py b/Examples/HelloGaussian.py
index 4dd90e9..75a194c 100644
--- a/Examples/HelloGaussian.py
+++ b/Examples/HelloGaussian.py
@e -7,5 +7,8 @e def p(x):
#let's plot it
x = np.linspace(-3,3,100)
y = p(x)
+print("I'm about to plot!")
plt.plot(x,y)
\ No newline at end of file
+plt.show()
[bash] Examples >
```



```
Examples - bash - 85x26
[bash] Examples > git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes not staged for commit:
 (use "git add <file>..." to update what will be committed)
  (use "ait checkout -- <file>..." to discard changes in working directory)
no changes added to commit (use "git add" and/or "git commit -a")
[bash] Examples > git add HelloGaussian.py
Γbashl Examples > □
```

```
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 Floation | Floating | Floati
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[bash] Examples > git add HelloGaussian.py
[bash] Examples > git commit -m "Added a print statement to the example"
[master 2358ef5] Added a print statement to the example
1 file changed, 4 insertions(+), 1 deletion(-)
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```

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On branch master
Your branch is ahead of 'origin/master' by 1 commit.
 (use "git push" to publish your local commits)
nothing to commit, working directory clean
Γbashl Examples >
```

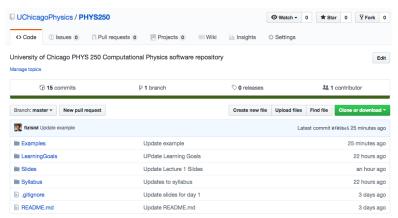
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nothing to commit, working directory clean
[bash] Examples > ait push -u
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```
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Your branch is ahead of 'origin/master' by 1 commit.
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nothing to commit, working directory clean
[bash] Examples > git push -u
Counting objects: 4. done.
Delta compression using up to 8 threads.
Compressing objects: 100% (4/4), done.
Writing objects: 100% (4/4), 402 bytes | 0 bytes/s, done.
Total 4 (delta 3), reused 0 (delta 0)
remote: Resolving deltas: 100% (3/3), completed with 3 local objects.
To https://aithub.com/UChicagoPhysics/PHYS250.ait
  0e29276..2358ef5 master -> master
Branch master set up to track remote branch master from origin.
[bash] Examples >
```

PHYS 250 GitHub

https://github.com/UChicagoPhysics/PHYS250

Course materials are hosted in the GitHub UChicagoPhysics repository



- Slides (e.g. these!), syllabi, learning goals, and code examples
- Stable versions will be cross-posted to Canvas as well.
- Homework submission will be done via **GitHub** (instructions to come)

GitHub & GitLab resources

In general, **GitHub** is a free resource as long as your code remains public (you can pay for private repositories). The Physical Sciences Division (PSD) at UChicago hosts a **private GitLab** repository.

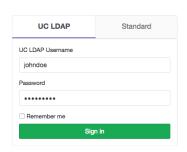
• https://psdcomputing.uchicago.edu/page/psd-repo



PSD Repo



PSD Repo is a software source code repository managed by the PSD Computing office



GitHub Education

However, there are a suite of resources available to you as students!

Real-world tools, engaged students

GitHub Education helps students, teachers, and schools access the tools and events they need to shape the next generation of software development.



GitHub Student Developer Pack The best developer tools, free for students



GitHub Campus Experts
Training to enrich the technology
community at your school



GitHub Field Day Unconferences for leaders of technical student communities



GitHub Classroom

The GitHub workflow, scaled for the needs of students



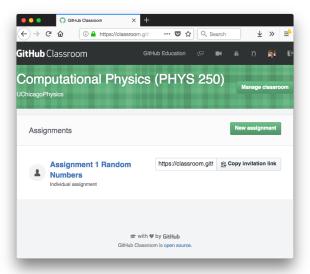
Advisors
Teacher training to master Git and GitHub

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- 2 Plan for homework
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- Physics
 - Random numbers: Introduction and motivation
 - Types of random numbers
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GitHub Classroom: assignments (I)

As mentioned on Tuesday, we will be using **GitHub** for distribution, assessment, and collection of assignments.



GitHub Classroom: assignments (II)

- You will receive a link to the assignment
- This provides your own unique respiratory based on a starter repository with examples and info that you might find useful for the assignment.
- The deadline will be **Thursday at 2pm**, at which time **GitHub** Classroom will save the latest commit from each repository as a submission.
- Submission commits are viewable **only to me and the TAs** on the assignment page.
- We can then make comments and grades directly on your submission.

For a tutorial about how this works, see this 3.5 min video:

https://youtu.be/rTsfBAV7sOo

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Random numbers

Random numbers may seem innocuous, but they underlie nearly everything you do electronically, rely on for security, or employ in the context of simulations and evaluation of models.

- cryptography
- computer simulation
 - most well-known of which is named after gambling town, Monte Carlo
- sampling

As such, their use, their control, and the evaluation of just how random they are, are of **paramount importance for computational physics.**

And you thought lava lamps were a thing of the past



Cryptography relies on the ability to generate random numbers that are both unpredictable and secret. But **random** is a very malleable term.

True vs. Pseudo: it's more than semantics

The computers of today are, by design and by implementation, *deterministic*. That means that an **algorithm cannot**, on its own and without input from an external source, provide a stream of 100% uncorrelated random sequences. Hence the division:

- TRNGs: True random number generators
 - generally use some physical process that is unpredictable, but often slow and requires specialized hardware
 - possibly combined with some compensation mechanism that might remove any bias in the process
 - examples include: lava lamps, quantum processes, radioactive decays, thermal noise
- PRNGs: Pseudo-random number generators
 - based on algorithms and, therefore, not truly random
 - do not require special hardware and therefore are very portable and fast
 - can be reproduced given initial conditions

We will, perhaps obviously, focus on PRNGs.

(but if you want to build a wall of lava lamps in KPTC, I will cheer you on)

Pseudo-random number generators (PRNGs)

The idea behind an algorithmic PRNG is to generate a sequence of numbers, x_1, x_2, x_3 ... using a recurrence of the form

$$x_i = f(x_{i-1}, x_{i-2}, ..., x_{i-n}),$$
 (1)

where n initial numbers ("seeds") are needed to begin the recurrence. The magic lies in the function, f, used, and the resulting *uniformity* and *correlation length* across some sequence of numbers.

Linear congruential generators (LCGs) are one of the oldest PRNGs and have the form

$$x_{i+1} = (ax_i + c) \mod m \tag{2}$$

IBM mainframes in the 60s had a = 65539, c = 0, and $m = 2^{31}$. This leads to

$$x_{i+2} = 6x_{i+1} - 9x_i (3)$$

which, maybe you can tell, isn't great.

Python random number generator: Mersenne Twister

Python has a built-in (stdlib) RNG that can be accessed with:

```
import random as rng
rng.random()
```

numpy has an even more developed set of tools with numpy.random.

```
from numpy import random as rng
rng.random()
```

Both of these use the Mersenne Twister algorithm, developed in 1997 by Matsumoto and Nishimura; is a version of a generalized feedback shift register PRNG. The name due to the fact that the period is given by a Mersenne prime (most commonly: n = 219937):

$$M_n = 2^n - 1, n \in \mathbb{N} \tag{4}$$

(In preparing this, I found out that the largest known prime number $2^{77,232,917} - 1$ is a Mersenne prime, found on December 26, 2017.)

Testing the true "randomness" of a RNG

Tests of RNGs must look for patterns in sequences of given lengths and frequencies and test those possible patterns against the probability that they occurred "accidentally" or whether they are happening more often than they should.

→ This brings us to our first example of **hypothesis testing**

Big business for RNGs:



See: https://www.random.org, http://www.cacert.org/, etc

Hypothesis testing

The most common **test statistic** is the chi-squared, χ^2

$$\chi^2 = \sum_{i=1}^n \frac{(O_i - E_i)^2}{E_i} = N \sum_{i=1}^n \frac{(O_i/N - p_i)^2}{p_i}$$
 (5)

where

- χ^2 = Pearson's cumulative test statistic, which asymptotically approaches a χ^2 .
- O_i = the number of observations of type *i*.
- N = total number of observations
- p_i = the fraction of type i w.r.t. the total (N)
- $E_i = Np_i$ = the expected (theoretical) count of type i
- n = the number of cells in the table.

This resembles a normalized sum of squared deviations between observed and theoretical frequencies of occurrence.

Hypothesis testing in our case

Instead of testing the **randomness** we can test the **uniformity** of our RNG using the χ^2 and a simple histogram:

$$\chi^2 = \sum_{i=1}^n \frac{(O_i - E_i)^2}{E_i} = N \sum_{i=1}^n \frac{(O_i/N - p_i)^2}{p_i}$$
 (6)

In the following, we can think of these quantities as:

- O_i = the number of times we get a number in some range (i.e. bin i of the histogram)
- N = total number of random numbers that we analyze
- p_i = the fraction of the total range of the random numbers that each bin i represents
- $E_i = Np_i$ = the expected number of times a random number lands in each bin i
- n = the number of bins in the histogram.

Testing the uniformity of this PRNG

A histogram is a graphical representation of a discrete probability distribution. To make a simple histogram, all you need to do is:

```
# Import the numpy random number generator
from numpy import random as rnq
# Import the plotting libraries
import matplotlib.pyplot as plt
 Generate 100 random nums
 distributed between [0,1)
 (returns a numpy array)
data = rnq.random(100)
# Fill a histogram
plt.hist(data)
plt.show()
```

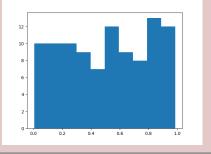
Testing the uniformity of this PRNG

A histogram is a graphical representation of a discrete probability distribution. To make a simple histogram, all you need to do is:

```
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from numpy import random as rng

# Import the plotting libraries
import matplotlib.pyplot as plt
```

```
# Generate 100 random nums
# distributed between [0,1)
# (returns a numpy array)
data = rng.random(100)
# Fill a histogram
plt.hist(data)
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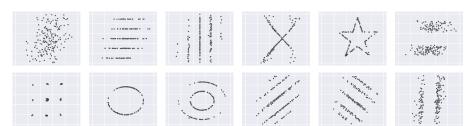


plt.show()

Words of caution regarding hypothesis testing and data sets

We want to compute a χ^2 to see if it's uniform (part of your homework assignment due next Thursday).

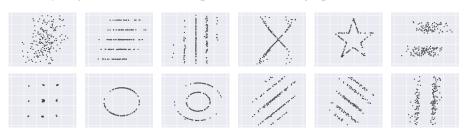
However, before going further: be **very wary of reliance on any one method** for analyzing a dataset. For example, look at these graphs:



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However, before going further: be **very wary of reliance on any one method** for analyzing a dataset. For example, look at these graphs:



As discussed in this paper, while different in appearance, each has the same summary statistics to 2 decimal places:

- means: $\bar{x} = 54.02, \bar{y} = 48.09$
- std. deviation: $\sigma_x = 14.52, \sigma_y = 24.79$
- Pearson's correlation coefficient: r = +0.32